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"ESSENTIALLY DISCONNECTED BENZENOIDS" ARE ESSENTIALLY DISCONNECTED

RONG–QIN SHENG[*], SVEN J. CYVIN[†] and IVAN GUTMAN[#]

[*] *Shanghai Institute of Computer Technology, 546 Yu Yuan Road, Shanghai, The People's Republic of China*

[†] *Division of Physical Chemistry, The University of Trondheim, N–7034 Trondheim–NTH, Norway*

[#] *Faculty of Science, University of Kragujevac, YU–34000 Kragujevac, Yugoslavia*

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Abstract

An essentially disconnected benzenoid system is defined as a Kekuléan benzenoid system which has fixed (single or double) bonds. It is described and strictly proved that the subgraph, obtained from an essentially disconnected benzenoid system by deleting all the fixed single bonds and all the end vertices of the fixed double bonds, is disconnected. This is just what the term "essentially disconnected" means. A necessary and sufficient condition for a benzenoid system to be essentially disconnected is given. Two procedures for obtaining all effective units are outlined.

1. Introduction

A benzenoid system is said to be Kekuléan if it possesses a Kekulé structure, otherwise non–Kekuléan. Essentially disconnected benzenoid systems are Kekuléan benzenoid systems with fixed bonds. Kekuléan benzenoid systems with no fixed bonds are called normal.

A fixed single (double) bond is an edge which corresponds to a single (double) bond in all Kekulé structures of a benzenoid system.

The term "essentially disconnected benzenoid" was used for the first time by Cyvin et al.[1]. A great number of examples [2] of essentially disconnected benzenoid systems have been found to have the essentially disconnected nature. This means that such a system consists of two ore more "effective units" being normal benzenoids, and a "junction". The junction is, by definition, the set of hexagons possessing fixed bonds. A general proof for the essentially disconnected nature of an essentially disconnected benzenoid has never been given before. In the present paper a rigorous proof to this effect is conducted.

Concerning the characterization of essentially disconnected benzenoid systems, Cyvin and Gutman [3] found some sufficient conditions for a benzenoid system to be essentially disconnected, but these conditions are not necessary. A structural characterization which amounts to a necessary and sufficient condition for a benzenoid system to be essentially disconnected has never been reported before. In the present paper we try to fill this gap. Two procedures for recognizing essentially disconnected benzenoid systems as well as detecting all the effective units are outlined.

2. Edge–cuts

In the present paper benzenoid systems are always oriented with some of their edges vertical.

Denote by $n^{(w)}(G)$ and $n^{(b)}(G)$ the numbers of white and black vertices in a colored bipartite graph G, respectively. Furthermore,

$$D(G) = n^{(b)}(G) - n^{(w)}(G). \tag{1}$$

Let B be a benzenoid system. In Ref. 4, an edge–cut of B was defined as a collection of edges $\mathbb{C}$ such that the subgraph B–$\mathbb{C}$ obtained from B by deleting all edges in $\mathbb{C}$ has more components than B. In the present paper, the definition of edge–cuts is restricted as follows:

Let B be a benzenoid system and $e_1,e_2,\ldots,e_t$ some of its edges. Then $\mathbb{C} = \{e_1,e_2,\ldots e_t\}$ is called an edge–cut of B if

(a) by deleting the edges $e_1,e_2,\ldots,e_t$ from B it decomposes into two parts B' and B";

(b) the black end vertex of e_i belongs to B' (and therefore the white end vertex of e_i belongs to B"), $i=1,2,\ldots,t$;

(c) each pair of edges e_i,e_{i+1}, $i=1,2,\ldots,t-1$, belongs to the same hexagon and e_1 and e_t belong to the perimeter.

LEMMA 1

If B is a Kekuléan benzenoid system and $\mathbb{C}$ one of its edge–cuts, then for each Kekulé structure of B the number of double bonds in $\mathbb{C}$ is an invariant, and is equal to $D(B')$; as a consequence, the edges in $\mathbb{C}$ are all fixed single bonds if and only if $D(B')=0$.

The above lemma can be easily verified [5].

Let $\mathbb{C}$ be an edge–cut of the benzenoid system B. Sometimes the value of $D(B')$ is also symbolized as $D(\mathbb{C})$:

$$D(\mathbb{C}) = D(B'). \tag{2}$$

An elementary edge–cut (EEC) is an edge–cut realized by a straight line segment (cut segment [5]) (see fig. 1).

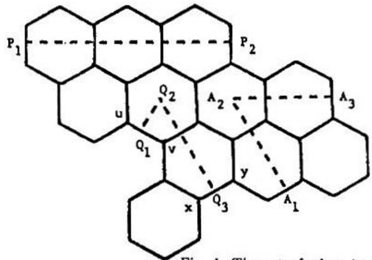

Fig. 1. The set of edges intersected by P_1P_2 is an EEC, the set of edges intersected by $A_1A_2A_3$ is a KEC. The set of edges intersected by $Q_1Q_2Q_3$ is a CKEC because u,v,x,y are all of degree three.

A K–edge–cut (KEC) is an edge–cut realized by a broken line segment consisting of two straight line segments which form an angle of 60° (see fig. 1) and intersect the perimeter only twice.

A characteristic K–edge–cut [6] (CKEC) is defined as a KEC in which the four end vertices of the two external edges are all of degree three (see fig. 1).

3. The essentially disconnected character of essentially disconnected benzenoid systems

LEMMA 2 (this lemma is well known in a more general context)

Let B be a Kekuléan benzenoid system, e an edge which is not a fixed bond, and K any Kekulé structure of B. Then there is in B a single–double alternating (conjugated) circuit which contains e.

Proof

There are Kekulé structures K_1, K_2 of B such that e is a single bond for K_1 and a double bond for K_2, where K equals K_1 or K_2. Consider the subgraph S of B generated by the edges which are single bonds for one of K_1, K_2 and double bonds for the other. Clearly, e belongs to S and every vertex of S has degree 2: thus the components of S are circuits, one of them – say, C – containing e. C is a conjugated circuit for K.

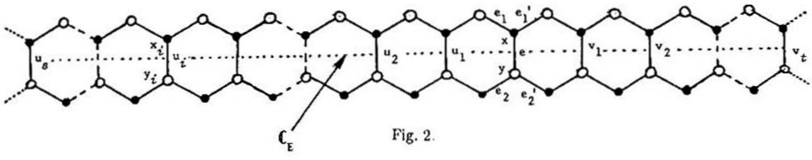

Fig. 2.

LEMMA 3

If B is an essentially disconnected benzenoid system with no fixed double bonds, then B has an EEC $\mathbb{C}_E$ for which $D(\mathbb{C}_E)=0$, or equivalently, the edges in $\mathbb{C}_E$ are all fixed single bonds.

Proof

Let e be a fixed single bond of B and $\mathbb{C}_E$ the EEC which contains e (see Fig. 2). We shall show that all edges in $\mathbb{C}_E$ are fixed single bonds.

B having no fixed double bonds, none of e_1, e_1', e_2, e_2', is a fixed bond. Let K be a Kekulé structure for which e_1 is a double bond and let C_1 be a conjugated circuit through e_1 (see Lemma 2). C_1 does not contain e_2 or e_2': suppose the contrary, then there is on C_1 a (directed) path P from x to y which starts and ends with a double bond (note that on P all edges from a black to a white vertex are double bonds), thus $P \cup \{e\}$ is a conjugated circuit – contradicting the hypothesis that e is fixed. So there are disjoint conjugated circuits C_1 through e_1 and C_2 through e_2, and we may assume that both e_1 and e_2 are double bonds. None of u_1, u_2, ..., u_s is a double bond since, otherwise, we find a conjugated circuit containing e (Fig. 3). Thus we have the situation of Fig. 4.

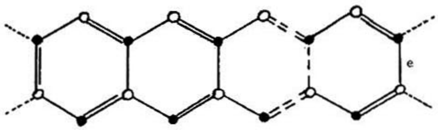

Fig. 3.

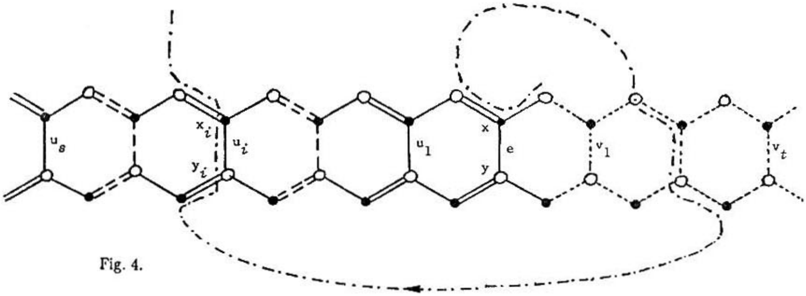

Fig. 4.

C_1 and C_2 do not contain any of the edges u_1, u_2, ..., u_s: suppose, w.l.o.g., that C_1 contains the edge u_i (see Fig. 4). Let P_1 be the path on C_1 starting from x with a double bond and terminating in x_i or y_i without containing u_i. Both of the first and the last edge of P_1 are double bonds, and as the first vertex is black, the last one must be white: thus P_1 cannot terminate in x_i. It cannot terminate in y_i either, by topological reasons (the circuit C_1 cannot intersect itself, see Fig. 4).

If we now interchange the single and double bonds on C_1 and C_2, we conclude in the same way that for the Kekulé structure $K^\star$ so obtained, v_1, v_2, ...,v_t are single bonds, and since u_1, u_2, ..., u_s remain single bonds for $K^\star$, all edges of $\mathbf{C}_E$ are single bonds for $K^\star$. By Lemma 1, all edges of $\mathbf{C}_E$ are fixed single bonds. ♦

LEMMA 4

Let B be a benzenoid system which has a vertical fixed double bond. Let e be a vertical fixed double bond such that no other vertical fixed double bond is above e. Let the upper vertex of e be incident to edge e_1 (and no other edge $\neq$ e) or to edges e_1, e_2 (Fig. 5). If e_1 lies on the boundary of B, then e_1 determines an EEC $\mathbf{C}_1$, all of whose edges being fixed single bonds. If e_1 does not lie on the boundary of B, then e_1 and e_2 determine a CKEC $\mathbf{C}^\star = \mathbf{C}_K$, all of whose edges being fixed single bonds (Fig. 6).

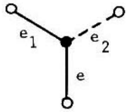

Fig. 5.

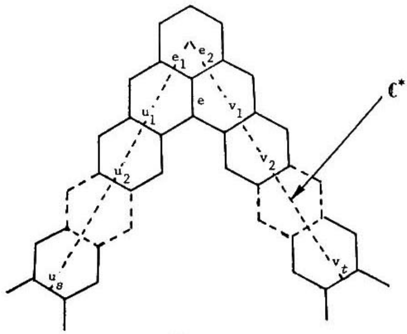

Fig. 6.

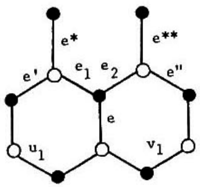

Fig. 7.

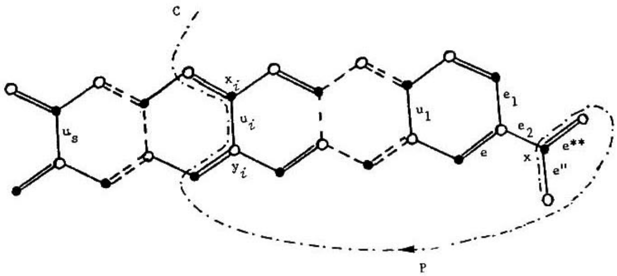

Fig. 8.

Proof

Consider Figure 7. e_1 is a fixed single bond. The edge e' must be present since $e^\star$ – if it exists – lies above e and, therefore, is not a fixed double bond. There is a Kekulé structure K such that e' is a double bond. Since e and e' are double bonds for K, we conclude as in the proof of Lemma 3 that all edges e_1, u_1, u_2, ... u_s are single bonds for K. If e_1 lies on the boundary of B, then this means that all edges of the EEC $\mathbb{C}_1$ are single bonds for K, implying (by Lemma 2) that all edges of $\mathbb{C}_1$ are fixed single bonds.

Now assume that e_1 does not lie on the boundary of B. Then e_2 exists and is a fixed single bond. The edges e_1 and e_2 determine a KEC $\mathbb{C}^\star$ (Fig. 6). If e'' is a double bond for K, then we conclude in the same way as above that also all edges v_1, v_2, ..., v_t are single bonds for K, implying that all edges of $\mathbb{C}^\star$ are fixed single bonds and, in addition, that $\mathbb{C}^\star$ is a CKEC.

If e'' is a single bond for K, then it cannot be a fixed bond since $e^{\star\star}$ (which lies above e, see Fig. 7) is not a fixed double bond. By Lemma 2, e'' lies on a conjugated circuit C. This circuit does not contain any of the edges u_1, u_2, ..., u_s. Suppose that C contains the edge u_i and no edge u_j with $j < i$ (see Fig. 8). Let P be the path on C starting from x with the double bond $e^{\star\star}$ and terminating in x_i or y_i without containing u_i. Both the first and the last edge of P are double bonds, and as the first vertex is white, the last one must be black; thus P cannot terminate in x_i. It cannot terminate in y_i either, by topological reasons (the circuit C cannot intersect itself; see Fig. 8.).

If we now interchange the single and double bonds on C, we conclude in the same way as above that for the Kekulé structure $K^{\star\star}$ so obtained, v_1, v_2, ..., v_t are single bonds, and since u_1, u_2, ..., u_s remains single bonds for $K^{\star\star}$, all edges of $\mathbb{C}$ are single bonds for $K^{\star\star}$. By Lemma 1, all edges of $\mathbb{C}^\star$ are fixed single bonds. Clearly, $\mathbb{C}^\star$ is a CKEC. ♦

THEOREM 1

If B is an essentially disconnected benzenoid system, then the subgraph from B obtained by deleting all fixed single bonds and all the end vertices of the fixed double bonds is disconnected.

Proof

According to Lemma 3 and Lemma 4, B has an EEC or a CKEC for which $D(B')=0$. There are two cases:

(i) For every EEC, $D(B')>0$. Let $\mathbb{C}'$ be an EEC through one of the highest lines of hexagons, then according to Lemma 4, any edge in $\mathbb{C}'$ is not a fixed double bond. Since $D(\mathbb{C}')=1$, $\mathbb{C}'$ contains an edge which is not a fixed bond. By the similar proof, an EEC $\mathbb{C}''$ through one of the lowest lines of hexagons contains an edge which is not a fixed bond. Then if $\mathbb{C}_K$ is a CKEC with $D(\mathbb{C}_K)=0$ (we may assume the edges in $\mathbb{C}_K$ are not vertical), consequently both B' and B" have an edge which is not a fixed bond.

(ii) There exists an EEC $\mathbb{C}_E$ such that $D(\mathbb{C}_E)=0$. We may assume the edges in $\mathbb{C}_E$ are vertical; the upper and lower parts are B' and B", respectively. We use K to designate the Kekulé structure count. See fig. 9, where the benzenoid system $B^\star$ contains B' and the hexagons which contain the edges in $\mathbb{C}_E$. The system B_1 is obtained by

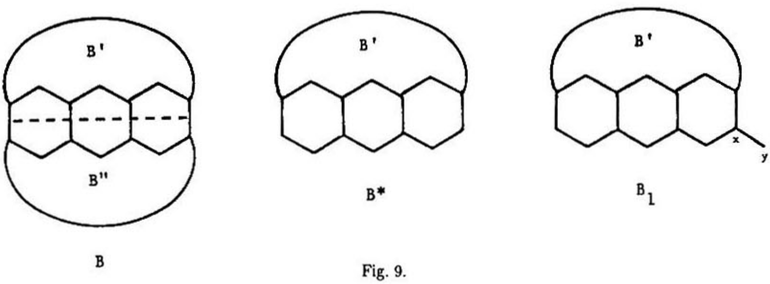

Fig. 9.

adding an edge {x,y} and a vertex y to $B^\star$, where x is the lower end vertex of an external edge in $\mathbf{C}_E$. It is easy to see that

$$K(B') = K(B_1). \tag{3}$$

Use the notation

$h^\star$=number of hexagons in $B^\star$,

$n^\star$=number of vertices of $B^\star$,

$n_i^\star$=number of internal vertices of $B^\star$.

Then [7,8]

$$n^\star = 4h^\star + 2 - n_i^\star. \tag{4}$$

In a Kekulé structure, the hexagon containing three double bonds is called an aromatic sextet. If B_1 has no aromatic sextets, then $B^\star$ contains $(n^\star-1)/2$ double bonds, the external edges of $B^\star$ contain $(n^\star-n_i^\star-2)/2$ double bonds at most, and thus the internal edges of $B^\star$ contain at least $(n_i^\star+1)/2$ double bonds. Consequently,

$$(n^\star-1)/2 \leq 2h^\star - (n_i^\star+1)/2 \ ,$$

i.e. $n^\star \leq 4h^\star - n_i^\star$, which contradicts the identity (4). Hence B_1 must contain an aromatic sextet, then $K(B_1) \geq 2$, and from (3) $K(B') \geq 2$. By the similar proof, $K(B'') \geq 2$. Therefore both B' and B" contain an edge which is not a fixed bond.

Consequently, the subgraph obtained from B by deleting all fixed single bonds and all end vertices of the fixed double bonds must have at least two components, and thus must be disconnected. This completes the proof. ♦

4. A necessary and sufficient structural requirement for a benzenoid system to be essentially disconnected

In a recent paper [6] by one of the present authors, a necessary and sufficient condition for a benzenoid system to be Kekuléan, which is stronger than that of Kostochka [9], was developed. According to Ref.6 a benzenoid system B is Kekuléan if and only if (i) $D(\mathrm{B})=0$, (ii) for every EEC and every CKEC, $D(\mathrm{B'})\geq 0$.

Then according to Lemma 3 and Lemma 4, we obtain

THEOREM 2

A benzenoid system B is essentially disconnected if and only if (i) $D(\mathrm{B})=0$, (ii) for every EEC and every CKEC, $D(\mathrm{B'})\geq 0$, (iii) there exists an EEC or a CKEC such that $D(\mathrm{B'})=0$.

THEOREM 2'

A benzenoid system B is normal if and only if (i) $D(\mathrm{B})=0$, (ii) for every EEC and every CKEC, $D(\mathrm{B'})>0$.

5. Two procedures for the effective units

According to Theorem 1, the subgraph obtained from an essentially disconnected benzenoid system B by deleting all fixed single bonds and all the end vertices of fixed double bonds is composed of m ($m\geq 2$) normal benzenoid units $\mathrm{B}_1,\mathrm{B}_2,\ldots,\mathrm{B}_m$, which are called effective units. Then a well known identity is that

$$K\{\mathrm{B}\} = \prod_{i=1}^{m} K\{\mathrm{B}_i\} \quad . \tag{5}$$

Two procedures for obtaining effective units are given in the following.

PROCEDURE 1

We are using Theorem 2. Let B be a benzenoid system with $D(\mathrm{B})=0$. For every EEC and every CKEC, calculate $D(\mathrm{B'})$. If $D(\mathrm{B'})<0$, then B is non–Kekuléan. If $D(\mathrm{B'})>0$ for all EEC's and CKEC's, then B is normal. If for some EEC or CKEC $D(\mathrm{B'})=0$, then delete all edges in the corresponding EEC or CKEC. After deleting all pendent vertices together with their first neighbours, the bridges as fixed single bonds and the end vertices of the bridges as fixed double bonds in the remaining part, continue with the components, and so on, until all remaining parts are normal benzenoids.

PROCEDURE 2

First by means of the algorithm of Sheng [10], rapidly judge whether B is Kekuléan. If B is Kekuléan, then a Kekulé structure drawn with single and double bonds is obtained at the same time. If $\mathbb{C}$ is an EEC or a CKEC, such that the edges in $\mathbb{C}$ are all single bonds, then delete all edges in $\mathbb{C}$. After deleting the cut–edges as fixed single bonds and the end vertices of the cut–edges as fixed double bonds in the remaining part, continue with components, and so on.

The Procedure 2 seems to be simple, and it is not necessary to determine the value $D(\mathrm{B}')$. It is a diagrammatical procedure.

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